checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

```
Bond precision:   C-C = 0.0182 A           Wavelength=1.54184

Cell:             a=18.4006(8)     b=11.9129(7)         c=13.0772(6)
                  alpha=90         beta=120.590(4)      gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           2467.6(2)                   2467.7(2)
Space group      C 2/c                       C 1 2/c 1
Hall group       -C 2yc                      -C 2yc
Moiety formula   C24 H16 Co N4 O4 S, 2(O)    ?
Sum formula      C24 H16 Co N4 O6 S          C24 H16 Co1 N4 O6 S1
Mr               547.40                      547.40
Dx,g cm-3        1.474                       1.473
Z                4                           4
Mu (mm-1)        6.655                       6.655
F000             1116.0                      1116.0
F000'            1111.22
h,k,lmax         20,13,14                    20,13,14
Nref             1925                        1900
Tmin,Tmax        0.480,0.553                 0.706,1.000
Tmin'            0.229

Correction method= # Reported T Limits: Tmin=0.706 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.987            Theta(max)= 61.730

                                                    wR2(reflections)=
R(reflections)= 0.1291( 1591)                       0.3236( 1900)
S = 6.379                  Npar= 164
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

```
EXPT005_ALERT_1_A  _exptl_crystal_description is missing
           Crystal habit description.
           The following tests will not be performed.
           CRYSR_01
GOODF01_ALERT_2_A  The least squares goodness of fit parameter lies
           outside the range 0.40 <> 6.00
           Goodness of fit given =      6.379
PLAT087_ALERT_2_A Unsatisfactory S value (Too High) .............       6.38 Check
PLAT430_ALERT_2_A Short Inter D...A Contact  O3       ..O3       .       1.91 Ang.
                                                1-x,y,1/2-z  =      2_655 Check
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value .......     Please Do !
```

Alert level B

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5712
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       2.97 eA-3
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......         O3 Check
PLAT341_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01825 Ang.
```

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C24 H16 Co N4 O6 S
             Rep.: C24 H16 Co1 N4 O6 S1
PLAT082_ALERT_2_C High R1 Value .................................       0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.32 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.08 Report
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/c       I2/a Note
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data     Please Note
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       2.16 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
```

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5 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
  7 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  3 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_EXPT005_I
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_GOODF01_I
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
_vrf_PLAT087_I
;
PROBLEM: Unsatisfactory S value (Too High) ..............       6.38 Check
RESPONSE: ...
;
```

```
_vrf_PLAT430_I
;
PROBLEM: Short Inter D...A Contact  O3       ..O3       .       1.91 Ang.
RESPONSE: ...
;
_vrf_PLAT699_I
;
PROBLEM: Missing _exptl_crystal_description Value .......     Please Do !
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock I - ellipsoid plot